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Phase Stability of Small Carbon Clusters[1] NICHOLAS WINTER, FRANCIS H. REE, Lawrence Livermore National Laboratory — The phase stability of nanometer size clusters of carbon atoms at high pressures and temperatures effects the detonation behavior of carbon-rich high explosives. Ab initio and semiempirical molecular orbital methods have been used to study the relative stability of carbon particles in the graphite and diamond phases as a function of cluster size. Calculations have also been carried out to characterize the influence of surface impurities (H, OH, N, etc.) on the phase stability.

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